

Interaction quench dynamics in the Kondo model in presence of a local magnetic field

M. Heyl and S. Kehrein

Department of Physics, Arnold Sommerfeld Center for Theoretical Physics and
Center for NanoScience, Ludwig Maximilians Universität München, Theresienstr. 37,
80333 Munich, Germany

E-mail: Markus.Heyl@physik.lmu.de

Abstract.

In this work we investigate the quench dynamics in the Kondo model on the Toulouse line in presence of a local magnetic field. It is shown that this setup can be realized by either applying the local magnetic field directly or by preparing the system in a macroscopically spin-polarized initial state. In the latter case, the magnetic field results from a subtlety in applying the bosonization technique where terms that are usually referred to as finite-size corrections become important in the present non-equilibrium setting. The transient dynamics is studied by analyzing exact analytical results for the local spin dynamics. The time scale for the relaxation of the local dynamical quantities turns out to be exclusively determined by the Kondo scale. In the transient regime, one observes damped oscillations in the local correlation functions with a frequency set by the magnetic field.

PACS numbers: 72.15.Qm, 71.27.+a

Submitted to: *J. Phys. C: Solid State Phys.*

1. Introduction

In recent years the possibility to experimentally study non-equilibrium dynamics in quantum many-body systems stimulated theoretical investigations of various model systems out of equilibrium. Of particular interest for this work is the observation that quantum dots can act as magnetic impurities displaying Kondo physics.[1] Due to the flexibility to vary system parameters in time by applying unscreened electrical or magnetic fields, quantum dots offer the framework for the experimental investigation of non-equilibrium dynamics in quantum impurity systems.

The Kondo model describes the physics of a localized spin $1/2$ coupled to a fermionic bath via an exchange interaction. At low temperatures, the sea of conduction band electrons develops a spin polarization cloud, the so-called Kondo cloud, providing a mechanism to screen the local magnetic moment. In the zero temperature limit, the screening becomes dominant leading to the emergence of the Kondo singlet such that the spin-polarization cloud is bound to the local spin with an associated binding energy T_K , the Kondo temperature. The Kondo effect manifests itself most prominently in the Kondo resonance, a sharp peak in the local density of states that is pinned at the Fermi energy.

As the Kondo model is the paradigm model for strongly correlated impurity systems, it is of particular interest that for a certain line in parameter space, the Toulouse limit, the Kondo model becomes exactly solvable by a mapping onto a quadratic resonant level model. [2, 3] In equilibrium as well as for an interaction quench, the Toulouse limit describes correctly many generic and universal properties of the Kondo model [3, 4, 5] such as the local spin dynamics that is also investigated in this work. Due to the complexity of time-evolution for systems out of equilibrium it is instructive to investigate those particular examples where exact and nonperturbative solutions are accessible.

Most of the work on time-dependent non-equilibrium systems has been concentrating on interaction quenches. [4, 5, 6, 7, 8, 9, 10, 11, 12] Due to its paradigmatic importance, the non-equilibrium quench dynamics in the Kondo model or the related Anderson impurity model in the local moment regime has been analyzed in a number of works. [4, 5, 6, 7, 8, 9, 10] Here, the transient dynamics in the Kondo model will be investigated for an interaction quench in presence of a local magnetic field. It will be shown that this scenario may be realized by either applying a local magnetic field directly or by preparing the system in a state in which the conduction band carries a macroscopic spin polarization. As the Kondo effect is sensitive to spin degeneracy, the local magnetic field is expected to influence the properties in the Kondo model considerably. The analysis of the transient dynamics and the emergence of the steady state will focus on the local spin dynamics as it is directly affected by the local magnetic field.

In the non-equilibrium setting where the lead carries a macroscopic initial spin polarization a subtlety in the application of the bosonization technique arises. Under certain circumstances as in this setting, terms that are usually referred to as finite-size

corrections may turn out to be relevant in the non-equilibrium case. As a consequence of the “finite size contributions” the spin-polarized initial state effectively acts as a local magnetic field applied to the local spin.

This paper is organized as follows. In Sec. II, the effective Hamiltonian for the dynamics in presence of a local magnetic field is derived. Afterwards, the magnetization of the impurity spin is investigated in Sec. III. Sec. IV is devoted to an analysis of the spin-spin correlation function and the results for the dynamical spin susceptibility are presented in Sec. V.

2. Effective Hamiltonian

The dynamics of a spin-1/2 coupled to a sea of electrons via an exchange interaction is described by the Kondo model:

$$H = \sum_{k\eta} k : c_{k\eta}^\dagger c_{k\eta} : + \sum_i \frac{J_i}{2} \sum_{\eta, \eta'} : \Psi_\eta^\dagger(0) \sigma_i^{\eta, \eta'} S_i \Psi_{\eta'}(0) :. \quad (1)$$

The operator $c_{k\eta}^\dagger$ creates an electron with wave vector k and spin $\eta = \uparrow, \downarrow$ in the reservoir. Here, we allow for an anisotropy in the exchange interaction resulting in different couplings in z-direction, $J_z = J_\parallel$, and in the xy plane, $J_x = J_y = J_\perp$. In the following, the couplings are all given in units of the noninteracting density of states. The colons $: \dots :$ denote normal ordering with respect to the Fermi sea. The local spin operator \vec{S} with components $S_i, i = x, y, z$, is coupled to the local spin density of the conduction band electrons whose components are determined by the Pauli matrices σ_i . The electron’s dispersion relation has been linearized around the Fermi level and energies are measured in units of v_F relative to the Fermi energy, i.e. $v_F = 1$ and $\varepsilon_F = 0$. As the local scatterer is assumed to be pointlike, only s-wave scattering occurs reducing the problem to a one-dimensional one. [3] For an additional magnetic field h_* applied to the local spin, the Hamiltonian in Eq. (1) acquires an extra contribution $-h_* S_z$.

In the following, we will work in the Toulouse limit of the Kondo model where the parallel coupling takes a special value $J_\parallel = 2 - \sqrt{2}$. The relevance of the Toulouse point in the single channel Kondo model is twofold. First, it allows for exact analytical results in a strongly correlated system. Secondly, the Toulouse point governs many generic and universal properties for the whole parameter regime including the experimentally relevant isotropic case. Especially, it has been shown that the local spin dynamics, that is also investigated in this work, shows the generic behavior in equilibrium as well as out of equilibrium. Other universal quantities, however, such as the Wilson ratio explicitly depend on the anisotropy.

In the following, two non-equilibrium scenarios will be investigated that turn out to induce the same dynamics. The first is an interaction quench in the Kondo model in presence of a magnetic field, i.e. the coupling J in the Kondo Hamiltonian is suddenly switched on while a local magnetic field is acting on the local spin. The second scenario investigates the dynamics in the Kondo model if the system is initially prepared in a state with a macroscopic spin polarization.

In equilibrium, the anisotropic Kondo Hamiltonian in the Toulouse limit can be mapped onto an exactly solvable resonant level model using bosonization and refermionization. [3] As has been shown by Lobaskin and Kehrein, such a mapping also exists in the case of an interaction quench where an additional local potential scattering term emerges. [4] Below, the implementation of the bosonization technique for the Kondo Hamiltonian with an applied local magnetic field will be presented. The bosonization technique is based on the bosonization identity

$$\psi_\eta(x) = \frac{1}{\sqrt{a}} F_\eta e^{-i\frac{2\pi}{L} N_\eta x} e^{-i\phi_\eta(x)}, \quad \eta = \uparrow, \downarrow, \quad (2)$$

that establishes a connection between fermionic fields $\psi_\eta(x)$ and bosonic fields $\phi_\eta(x)$ as an elementary operator identity in Fock space, see Ref. [13] for a recent review. Here, $\phi_\eta(x) = -\sum_{q>0} [e^{-iqx} b_{q\eta} + e^{iqx} b_{q\eta}^\dagger] e^{-aq/2} / \sqrt{n_q}$, $b_{q\eta} = -i/\sqrt{n_q} \sum_k c_{k-q\eta}^\dagger c_{k\eta}$, $q = 2\pi n_q/L$ with $n_q \in \mathbb{N}$, L is the system size and $a^{-1} > 0$ is an ultraviolet cutoff. The Klein factor F_η accounts for the annihilation of one electron as this cannot be accomplished by the bosonic field $\phi_\eta(x)$.

As usual, the bosonized Hamiltonian in the Toulouse limit can be simplified tremendously by applying a sequence of unitary transformations. First, the charge and spin (c,s) degrees of freedom are separated by introducing $\phi_{c/s}(x) = \frac{1}{\sqrt{2}} [\phi_\uparrow(x) \pm \phi_\downarrow(x)]$, $\hat{N}_{c/s} = \frac{1}{2} [\hat{N}_\uparrow \pm \hat{N}_\downarrow]$. The charge sector decouples from the impurity problem and will be neglected in the following.

In the Toulouse limit where $J_\parallel = 2 - \sqrt{2}$, the Emery-Kivelson transformation $U = e^{i[\sqrt{2}-1]\phi_s(0)[S_z-1/2]}$ eliminates the many-body interaction term in the Kondo Hamiltonian that couples to the S_z operator. Refermionization of the transformed Hamiltonian reduces the problem to a quadratic and therefore exactly solvable one. For that purpose, another unitary transformation $U_2 = e^{i\pi \hat{N}_s S_z}$ has to be imposed. [14] This allows to define the fermionized spin operator $d = e^{-i\pi[\hat{N}_s - S_z]} S_-$ and its hermitian conjugate d^\dagger as well as new spinless fermionic fields

$$\psi(x) = \frac{1}{\sqrt{a}} F_s e^{-i\frac{2\pi}{L} \hat{N}_s x} e^{-i\phi_s(x)}, \quad F_s = F_\downarrow^\dagger F_\uparrow, \quad (3)$$

with modes $c_k = (2\pi L)^{-1/2} \int dx e^{ikx} \psi(x)$. In the case of an applied local magnetic field h_* , an additional contribution $-h_* S_z$ appears in the Hamiltonian. The S_z operator commutes with the unitary transformations U and U_2 and can be related to the fermionic d operators in the following way:

$$S_z = d^\dagger d - \frac{1}{2}. \quad (4)$$

Thus, a local magnetic field induces a shift of the energy of the d fermion. After the mapping, the effective Hamiltonian reduces to a noninteracting resonant level model with an additional local scatterer:

$$\begin{aligned} H_{\text{eff}} = & \sum_k k :c_k^\dagger c_k: - \varepsilon_0 d^\dagger d + g \sum_{kk'} :c_k^\dagger c_{k'}: \\ & + V \sum_k \left[c_k^\dagger d + d^\dagger c_k \right] + \Delta E \end{aligned} \quad (5)$$

where $V = J_\perp \sqrt{\pi/(2aL)}$, $g = [\sqrt{2} - 1]\pi/L$, $\varepsilon_0 = h_*$ and ΔE denotes a constant energy shift. The magnetic field solely enters the Hamiltonian by shifting the local d level ε_0 away from the Fermi level.

The Kondo scale can be related to parameters of the resonant level model Hamiltonian by the impurity contribution to the Sommerfeld coefficient in the specific heat: [4] $C_{\text{imp}} = \gamma_{\text{imp}} T$ with $\gamma_{\text{imp}} = w\pi^2/3T_K$. Here, $w = 0.4128$ is the Wilson number. In this way the Kondo temperature is determined by $T_K = \pi w \Delta$ where $\Delta = V^2 L/2$.

As will be shown in the following, a Hamiltonian of the same structure as in Eq. (5) is induced by preparing the system in a state with a macroscopic spin polarization:

$$|\psi_0\rangle = \prod_{0 < k < k_*} c_{k\uparrow}^\dagger |0\rangle \otimes |\chi\rangle. \quad (6)$$

Here, $|0\rangle$ is the filled Fermi sea and $|\chi\rangle$ a wave function for the local spin. For simplicity, we set the initial spin wave function $|\chi\rangle = |\uparrow\rangle$ in the following. The wave vector k_* denotes the electronic state up to which the spin up electrons are filled. Indeed, the state $|\psi_0\rangle$ carries a macroscopic spin polarization:

$$\hat{N}_s |\psi_0\rangle = \frac{L}{4\pi} k_* |\psi_0\rangle. \quad (7)$$

The operator $\hat{N}_s = [\hat{N}_\uparrow - \hat{N}_\downarrow]/2$ measures the total spin of the conduction band electrons.

Note, that Kondo impurities attached to ferromagnetic leads [15] describe a different setup, as there the chemical potentials for the up and down spin electron species are identical, whereas the corresponding densities of states are different. Here, the chemical potentials differ in the initial state and it is assumed that the densities of states are identical by choosing the same Fermi velocities for the up and down spin electrons. This is reasonable as long as the wave vector k_* is small enough in order to neglect the influence of curvature on the dispersion relation.

Using the bosonization technique for the mapping onto a quadratic effective Hamiltonian, it is important to recognize that expressions like

$$\lim_{L \rightarrow \infty} \frac{2\pi}{L} \hat{N}_s \neq 0 \quad (8)$$

do not vanish in the thermodynamic limit due to the macroscopic initial spin polarization. Those terms usually appear as finite-size corrections when expressing the fermionic density in terms of the bosonic fields and the number operators and cannot be neglected in the present study. As has been shown recently, the application of the bosonization technique requires additional effort in non-equilibrium scenarios. [16, 17] The implications of Eq. (8) will be studied in the following for the kinetic energy of the spin sector H_{0s} that equals in terms of the bosonic field ϕ_s and the number operator \hat{N}_s :

$$H_{0s} = \int dx \frac{1}{2} : (\phi_s(x))^2 : + \frac{2\pi}{L} \hat{N}_s^2. \quad (9)$$

Due to the spin-conservation condition [14]

$$S_T = \hat{N}_s + S_z = \text{const.} = \frac{L}{4\pi} k_* + \frac{1}{2} \xrightarrow{L \rightarrow \infty} \frac{L}{4\pi} k_* \quad (10)$$

one can express the latter term of the right-hand side in Eq. (9) in terms of the total spin S_T and the S_z operator such that:

$$\frac{2\pi}{L}\hat{N}_s^2 = \frac{2\pi}{L}S_T^2 - k_*S_z + \frac{\pi}{2L} = -k_*S_z + \text{const.} \quad (11)$$

Here, the identity $S_z^2 = 1/4$ has been used. Only in the case of a macroscopic spin-polarized initial state, one therefore obtains an additional non-vanishing contribution that is equivalent to a magnetic field of strength k_* applied to the local spin. As in this example, the operator \hat{N}_s can always be converted into a constant and the local spin operator S_z generating new terms in the Hamiltonian compared to the equilibrium or interaction quench case without magnetic field. In the end one arrives at an effective Hamiltonian that is equal to Eq. (5) with $\varepsilon_0 = \frac{2\pi}{L}[1 - J_{\parallel}]S_T = [\sqrt{2} - 1]k_*/2$

As shown in Appendix A, the occupation distribution $f_k = \langle \psi_0 | c_k^\dagger c_k | \psi_0 \rangle$ of the spinless fermionic operators in the initial state equals:

$$f_k = \theta\left(\frac{k_*}{2} - k\right). \quad (12)$$

The chemical potential $k_*/2$ in the initial state can be compensated by defining new operators $a_k = c_{k-k_*/2}$ in terms of which the structure of the effective Hamiltonian does not change. All c_k operators are replaced by a_k 's, only the energy of the local level gets modified to $\tilde{\varepsilon}_0 = k_*/\sqrt{2}$. Therefore, the initial state effectively acts as a magnetic field of strength:

$$h_* = \frac{k_*}{\sqrt{2}}. \quad (13)$$

Notice that the magnetic field seen by the impurity spin depends on J_{\parallel} , that characterizes the strength of the coupling between the z component of the local spin and the z component of the spin-polarization cloud generated by the itinerant electrons. In the Toulouse limit, the parallel coupling is fixed to a comparatively large value $J_{\parallel} = 2 - \sqrt{2}$. We expect, however, that independent of the actual coupling strength and away from the Toulouse limit the spin-polarized initial state always acts as a local magnetic field. Moreover, even in the limit $J_{\parallel} \rightarrow 0$, there is an effective magnetic field stemming from the kinetic energy of the spin sector, see. Eq. (11). The only relevant quantity is the total effective magnetic field h_* seen by the impurity spin.

Concluding, it has been shown that the dynamics in the Kondo model for an initially spin-polarized state of the type in Eq. (6) is equivalent to an interaction quench in presence of a magnetic field, see Eq. (5).

3. Magnetization

The local spin dynamics for an interaction quench in the Kondo model without magnetic field is well studied in the literature. In such a scenario, the magnetization $P_{h_*=0}(t) = \langle S_z(t) \rangle_{h_*=0}$ of the impurity spin [4, 3, 10, 18]

$$P_{h_*=0}(t) = P(0) e^{-2\Delta t} \quad (14)$$

decays to zero exponentially fast on a time scale $1/2\Delta$ that is set by the Kondo time scale $t_K = 1/T_K = 1/(\pi w\Delta)$.

As the local spin is sensitive to a local magnetic field, one expects that the magnetization dynamics differs considerably compared to the interaction quench case. Due to Eq. (4), the magnetization $P(t)$ is equivalent to the local d level occupation $\hat{n}_d = d^\dagger d$ up to a constant:

$$P(t) = \langle \hat{n}_d(t) \rangle - \frac{1}{2}. \quad (15)$$

As the effective Hamiltonian in Eq. (5) is quadratic, the time evolution of the single-particle operators c_k and d is entirely determined by the Green's functions $G_W(t) = \theta(t)\langle \{c_l(t), c_{l'}\} \rangle$:

$$c_l(t) = \sum_{l'} G_W(t) c_{l'}, \quad l, l' = k, d \quad (16)$$

where G is a unitary matrix. The Green's functions $G_W(t)$ can be obtained by using the equations of motion approach, for example. As a result, one obtains for the magnetization of the impurity spin:

$$P(t) = \frac{1}{2} [1 + \Lambda(0)] e^{-2\Delta t} - e^{-\Delta t} \Lambda(t) + \frac{1}{2} \Lambda(0) \quad (17)$$

where $\Lambda(t) = (2/\pi) \int_0^{h_*/\Delta} d\omega \cos(\omega\Delta t)/(1 + \omega^2)$ and $\Lambda(0) = (2/\pi) \text{atan}(h_*/\Delta)$. Notice that this agrees with the result in Eq. (14) in the limit $h_* \rightarrow 0$ as expected. Plots of the magnetization for different values of the magnetic field h_* are shown in Fig. 1. As one can see, the time scale for relaxation of the magnetization is exclusively set by the Kondo scale t_K independent of the magnetic field. For the local level occupation in an interaction quench in a Majorana resonant level model, the equivalent relaxation behavior has been observed in a recent work by Komnik. [12] The time scale $t_* = 1/h_*$ associated with the magnetic field dominates the transient dynamics as long as $t_* < t_K$, i.e. the magnetic field $h_* > T_K$ is sufficiently large.

As the curves in Fig. 1 indicate, the initial decay of the magnetization is universal in the sense that it is independent of the magnetic field or equivalently the initial spin polarization and exactly equals the interaction quench case:

$$\langle S_z(t) \rangle \stackrel{t \ll t_*, t_K}{\approx} \frac{1}{2} - \Delta t + \mathcal{O}(t^2). \quad (18)$$

The impurity spin is flipped without recognizing the presence of the magnetic field or the spin-polarized lead at short times. Approaching the time scale t_* , one observes a deviation from this universal initial decay and $P(t)$ reaches its minimum leading to overshooting. For sufficiently large magnetic fields $h_* > T_K$ and for times $t > t_*$, damped oscillations appear and the magnetization finally saturates at a value $P(t = \infty) = \pi^{-1} \text{atan}(h_*/\Delta)$, that is the equilibrium value of the magnetization in the Kondo model with an applied magnetic field h_* .

In terms of the initial spin polarization, the finite asymptotic value of the magnetization indicates that the impurity is not able to depolarize the system although

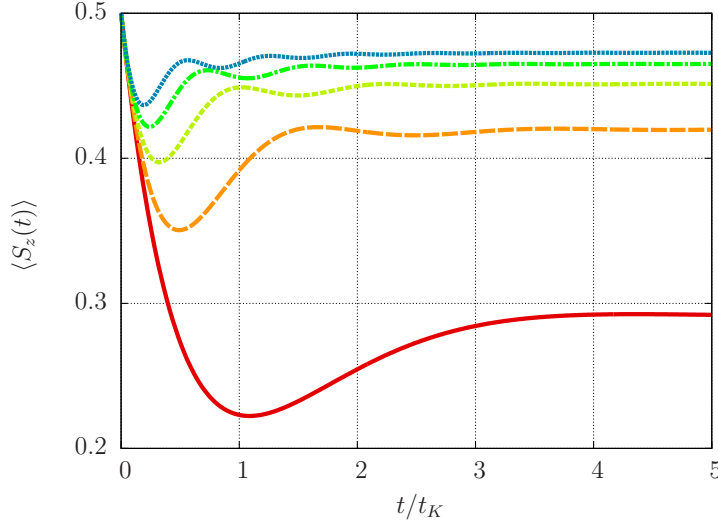


Figure 1. Magnetization $P(t) = \langle S_z(t) \rangle$ for different values of the local magnetic field $h_*/T_K = 9, 7, 5, 3, 1$ from top to bottom.

it can flip spins. Due to spin conservation, compare Eq. (10), the subspace of the total Hilbert space \mathcal{H}_{dyn} that is accessible by the dynamics can be restricted to:[14]

$$\mathcal{H}_{\text{dyn}} = \mathcal{H}_+ \oplus \mathcal{H}_- \quad (19)$$

where the subspaces \mathcal{H}_{\pm}

$$\begin{aligned} \mathcal{H}_+ &= \text{span} \left[\left| S_T + \frac{1}{2}, \downarrow \right\rangle \right], \\ \mathcal{H}_- &= \text{span} \left[\left| S_T - \frac{1}{2}, \uparrow \right\rangle \right] \end{aligned} \quad (20)$$

contain those states that have a sea of conduction band electrons with spin $S_T \pm \frac{1}{2}$ and a local spin on the impurity with spin \downarrow, \uparrow . The impurity is therefore able to flip spins, the spin conservation condition, however, limits the maximally possible induced change of spin in the conduction band to one spin flip process from spin-up to spin-down such that the impurity is not able to compensate for the macroscopic initial spin polarization.

For large magnetic fields, $h_* \gg T_K$, the magnetization for times $t \gg t_* = 1/h_*$

$$\delta P(t) \xrightarrow{h_* \gg T_K} \left[\Lambda(0) - \frac{1}{2} \right] e^{-2\Delta t} - \frac{2\Delta}{\pi h_*} \frac{\sin(h_* t)}{h_* t} e^{-\Delta t} \quad (21)$$

reveals the frequency $\Omega_* = h_*$ of the oscillations in the magnetization that can be clearly seen in Fig. (1). Here $\delta P(t) = P(t) - P(t = \infty)$ denotes the deviation from the asymptotic equilibrium value $P(t = \infty)$.

For arbitrary fields $h_* \neq 0$, the asymptotic long-time behavior of the magnetization

$$\delta P(t) \xrightarrow{t \gg t_*, t_K} -\frac{2}{\pi} \frac{\Delta^2}{\Delta^2 + h_*^2} \frac{\sin(h_* t)}{\Delta t} e^{-\Delta t} \quad (22)$$

changes significantly compared to the interaction quench case without magnetic field, see Eq. (14), where it is exponential with rate 2Δ . Even a small magnetic field slows

down the decay. It becomes exponential at a rate Δ times an algebraic contribution proportional to $(\Delta t)^{-1}$. Recently, a similar slow asymptotic decay for the magnetization in presence of a magnetic field was found in the work by Ratiani and Mitra [9] where the transient dynamics in a quench from a single to a two-channel Kondo model has been studied. Regarding Eq. (22), in the limit $h_* \rightarrow 0$ the asymptotic long-time behavior of the magnetization crosses over into the interaction quench dynamics without magnetic field, compare Eq. (14), since the prefactor vanishes. The decay becomes proportional to $e^{-2\Delta t}$ as one can see from Eq. (17) with $\Lambda(t) = 0$ for $h_* = 0$.

In equilibrium as well as for an interaction quench, it has been shown that the Toulouse limit of the Kondo model describes qualitatively correct the dynamics of the local spin observables. [3, 4, 5] One may raise the question whether this extends to the present case with an additional magnetic field. In a recent work, Anders and Schiller [7] determined the magnetization for the same setup in the experimentally relevant case of an isotropic Kondo model at small couplings using the time-dependent numerical renormalization group technique. Comparing their numerically exact results with the analytical treatment shown here one finds very good qualitative agreement. As in the present Toulouse limit analysis, they observe an initial universal decay. Approaching $t \sim t_*$, the magnetization develops a minimum and damped oscillations appear for $t > t_*$ as long as the magnetic field is sufficiently large. The magnetization relaxes on the time scale t_K to a finite asymptotic value. Those main features all appear in the present analysis such that one can expect that the behavior of the other local dynamical quantities such as the spin-spin correlation function and the dynamical spin susceptibility obtained on the Toulouse line are describing qualitatively the correct behavior for the isotropic Kondo model at small couplings.

4. Spin-spin correlation function

Additional information about the local dynamical properties of the system is contained in the spin-spin correlation function

$$\langle S_z(t)S_z(t_w) \rangle = C(t, t_w) - \frac{i}{2}\chi(t, t_w) \quad (23)$$

that probes the correlation between two spin measurements at different times. Its real part $C(t, t_w) = \frac{1}{2}\langle \{S_z(t), S_z(t_w)\} \rangle$ is connected to the strength of the spin fluctuations and its imaginary part determines the response function $\chi(t, t_w) = i\theta(t - t_w)\langle [S_z(t), S_z(t_w)] \rangle$ for times t bigger than the waiting time t_w .

Due to Eq. (4), the spin-spin correlation function can be related directly to operators of the effective Hamiltonian:

$$\langle S_z(t)S_z(t_w) \rangle = \langle \hat{n}_d(t)\hat{n}_d(t_w) \rangle - \frac{1}{2}[P(t) + P(t_w)] - \frac{1}{4}. \quad (24)$$

From the evaluation of $\langle \hat{n}_d(t)\hat{n}_d(t_w) \rangle$ one obtains for the cumulant $\langle S_z(t)S_z(t_w) \rangle_C = \langle S_z(t)S_z(t_w) \rangle - \langle S_z(t) \rangle \langle S_z(t_w) \rangle$ of the spin-spin correlation function:

$$\langle S_z(t)S_z(t_w) \rangle_C = \Omega(t, t_w) [\Lambda(t - t_w) - e^{-\Delta t}\Lambda(t_w) -$$

$$-e^{-\Delta t_w} \Lambda(t) + e^{-\Delta(t+t_w)}(1 + \Lambda(0)) + \Omega(t, t_w)] \quad (25)$$

where the function Ω is given by:

$$\Omega(t, t_w) = \frac{1}{\pi} \int_{h_*/\Delta}^{\infty} d\omega \frac{[e^{-i\omega\Delta t} - e^{-\Delta t}][e^{i\omega\Delta t_w} - e^{-\Delta t_w}]}{1 + \omega^2}. \quad (26)$$

One fundamental question connected to non-equilibrium quench dynamics concerns the thermalization behavior of observables. [4, 5, 11, 6, 7, 8, 9] As for the magnetization, the relaxation of the spin-spin correlation function happens exponentially fast on a time scale $1/\Delta \propto t_K$ set by the Kondo scale with a further suppression by an additional algebraic contribution $(\Delta t_w)^{-1}$:

$$\delta\langle S_z(t + t_w) S_z(t_w) \rangle \xrightarrow{t_w \gg t_*, t_K} F(t, t_w) \frac{e^{-\Delta t_w}}{\Delta t_w}. \quad (27)$$

Here, $\delta\langle S_z(t + t_w) S_z(t_w) \rangle = \langle S_z(t + t_w) S_z(t_w) \rangle - \langle S_z(t) S_z \rangle_{eq}^{h_*}$ denotes the deviation of the spin-spin correlation function from its asymptotic relaxed form which is just the equilibrium spin-spin correlation function $\langle S_z(t) S_z \rangle_{eq}^{h_*}$ with applied magnetic field h_* . The function $F(t, t_w)$ is an oscillating function of t_w with period $2\pi/h_*$ and does not contribute to the relaxation dynamics. Comparing Eq. (27) with the result for an interaction quench obtained by Lobaskin and Kehrein [4], one observes that the relaxation behavior of the spin-spin correlation function does not change considerably. The magnetic field only leads to a modification of the function $F(t, t_w)$. As already observed for the magnetization, the time scale for thermalization of the spin-spin correlation function is exclusively set by the Kondo scale t_K .

In equilibrium at zero temperature without magnetic field, the spin-spin correlation function shows a universal algebraic long-time behavior [3]

$$\langle S_z(t) S_z \rangle_{eq} \xrightarrow{t \gg t_K} -\frac{1}{[\pi \Delta t]^2}. \quad (28)$$

In the present non-equilibrium setting, the universal long-time behavior remains unchanged:

$$\begin{aligned} \langle S_z(t) S_z(t_w) \rangle_C &\xrightarrow{t \gg t_K, t_*, t_w} -\left[\frac{\Delta^2}{h_*^2 + \Delta^2} \right]^2 \times \\ &\times \frac{1 - 2 \cos(h_* t_w) e^{-\Delta t_w} + e^{-2\Delta t_w}}{[\pi \Delta (t - t_w)]^2} \end{aligned} \quad (29)$$

with only a different prefactor. This universality originates from the property of the spin-spin correlation function that its asymptotic long-time behavior is solely dependent on the low-energy excitations in the vicinity of the Fermi level as one can show by a simple Fermi liquid argument. In equilibrium, one can expand the d operator in the energy representation of operators a_ε that diagonalize the Hamiltonian in Eq. (5), such that one obtains:

$$d = \rho_0^{-1/2} \sum_{\varepsilon} f_{\varepsilon} a_{\varepsilon}. \quad (30)$$

Here, $|f_\varepsilon|^2$ is the local single-particle density of states $\rho_d(\varepsilon)$ of the effective Hamiltonian at energy ε and $\rho_0 = L/(2\pi)$ is the noninteracting density of states of the lead. In the energy representation, the spin-spin correlation function then reduces to:

$$\langle S_z(t)S_z \rangle_{eq} = \left[\rho_0^{-1} \sum_{\varepsilon>0} |f_\varepsilon|^2 e^{-i\varepsilon t} \right]^2. \quad (31)$$

Performing a Wick rotation $t \rightarrow -i\tau$, one observes that for large τ only the low energy states contribute. Assuming that $|f_\varepsilon|^2$ is well behaved near the Fermi level $\varepsilon = 0$ such that it may be expanded around $\varepsilon = 0$ and replacing τ by it , the long-time behavior of the spin-spin correlation function is given by:

$$\langle S_z(t)S_z \rangle_{eq} \xrightarrow{t \rightarrow \infty} \left[\frac{\rho_d}{it} \right]^2. \quad (32)$$

In equilibrium at zero magnetic field, the local level $\varepsilon_0 = 0$ exactly lies at the Fermi energy such that the local density of states ρ_d at the Fermi level equals $\rho_d = 1/(\pi\Delta)$ and the exact result of Eq. (28) is reproduced. In case of an applied magnetic field h_* , the local d level is shifted away from the Fermi energy leading to a reduction of the local density of states $\rho_d = (\Delta/\pi)/(\Delta^2 + h_*^2)$. Comparing with the result in Eq. (29), one observes that the prefactor in the long-time behavior of the relaxed spin-spin correlation function for $t_w \rightarrow \infty$ exactly equals the square of the local density of states as expected from the Fermi liquid argument above.

For intermediate waiting times $0 < t_w < \infty$, the long-time behavior acquires a modification by damped oscillations with period $2\pi/h_*$ as a function of the waiting time t_w . This is a consequence of the transient non-equilibrium state where the Fermi liquid argument is not valid. At zero waiting time $t_w = 0$, the decay becomes exponential as the initial state is an eigenstate of the S_z operator and the spin-spin correlation function reduces to the magnetization of Sec. III as has been observed for the case of an interaction quench without magnetic field. [4]

5. Dynamical spin susceptibility

The imaginary part of the spin-spin correlation function determines the response of the system to a small external magnetic field $h(t)$ applied to the local spin. In the linear response regime, the magnetization in presence of $h(t)$ equals:

$$\langle S_z(t) \rangle_h = \langle S_z(t) \rangle + \int_{-\infty}^{\infty} dt' \chi(t, t') h(t'). \quad (33)$$

Expectation values without an index h are to be evaluated with the unperturbed Hamiltonian. In equilibrium, the response function depends only on the time difference thereby establishing a spectral representation in terms of one frequency. Its imaginary part $\chi''(\omega)$, the dynamical spin susceptibility, shows a peak near the Kondo temperature representing the Kondo singlet. In the non-equilibrium setting considered in this work,

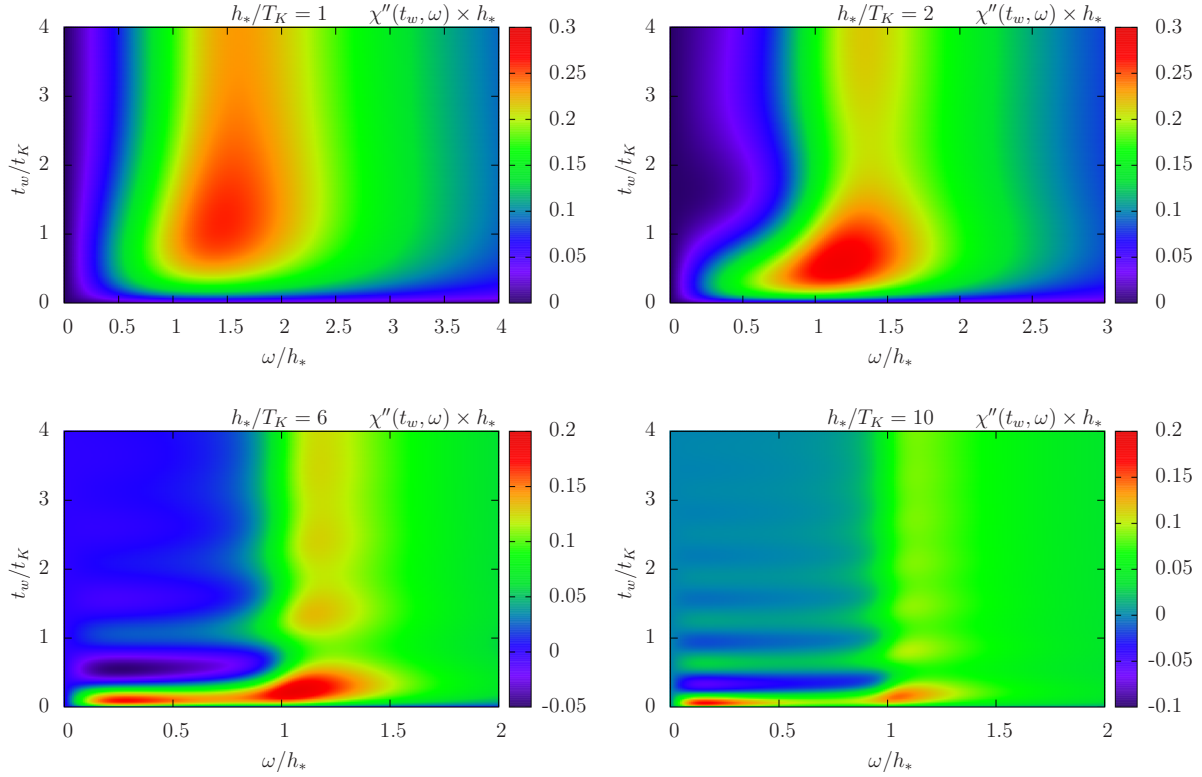


Figure 2. False color plots of the dynamical spin susceptibility $\chi''(t_w, \omega)$ for different values of the magnetic field h_* .

the suitable generalization of the spectral representation of the response function is the following: [4]

$$\chi(t_w, \omega) = 2 \int_0^\infty \frac{dt}{2\pi} e^{i\omega t} \chi(t + t_w, t_w). \quad (34)$$

The integration is only taken over the positive real axis as a consequence of causality such that an additional prefactor of 2 is required in order to reproduce the equilibrium case. The function $\chi(t_w, \omega)$ may be interpreted as the spectral decomposition of the response function at a given point t_w in time. Accordingly, $\chi''(t_w, \omega) = \text{Im}\chi(t_w, \omega)$ determines the dynamical spin susceptibility at a given point t_w in this non-equilibrium setup. False color plots of $\chi''(t_w, \omega)$ are shown in Fig. 2 for different degrees of initial spin polarization.

As one can see from Fig. 2, the time scale for relaxation of the dynamical spin susceptibility is solely determined by the Kondo scale t_K as already found for the magnetization and the spin-spin correlation function.

For small magnetic fields $h_* < T_K$, the behavior of the dynamical spin susceptibility resembles the interaction quench case without magnetic field. In the transient regime up to times $t \sim t_K$, the dynamical spin susceptibility approaches its equilibrium shape exponentially fast with a peak located at $\omega \approx T_K$ associated with the Kondo singlet as one observes in the case without magnetic field. [6, 4]

For magnetic fields $h_* \gtrsim T_K$, as can be seen in the plots of Fig. 2, a maximum builds up on a time scale t_* whose position roughly scales proportional to the magnetic field. Importantly, the peak associated with the Kondo singlet near T_K is not visible any more indicating that the large magnetic field avoids the buildup of Kondo correlations. The spin fluctuations that are the basis for the emergence of the Kondo effect are suppressed as the impurity spin is pinned by the strong magnetic field. After a fast initial buildup on a time scale t_* associated with the initial spin polarization, damped oscillations appear in the dynamical spin susceptibility with frequency h_* decaying on a scale t_K .

6. Conclusions

In this work, the quench dynamics of the Kondo model in the Toulouse limit has been analyzed in presence of a local magnetic field. It has been shown that this setup can be realized either by applying the magnetic field directly or by preparing the system in a macroscopically spin-polarized state. The effective magnetic field caused by the initial state results from a subtlety in applying the bosonization technique. Terms that are usually referred to as finite-size corrections become important in this non-equilibrium setting. The transient dynamics has been investigated by analyzing exact analytical results for the local spin dynamics such as the magnetization, the spin-spin correlation function and the dynamical spin susceptibility.

The analysis revealed that the time scale for relaxation of all the investigated local dynamical quantities is exclusively set by the Kondo scale t_K and is independent of the magnetic field h_* , compare Eqs. (14), (27) and Fig. (1), (2).

The magnetization shows damped oscillations with a frequency h_* set by the magnetic field for $h_* > T_K$. Compared to the interaction quench case without magnetic field, the asymptotic long-time decay of the magnetization becomes slower in the present setup with a different scaling behavior, compare Eq. (22). Overall, the analysis of the magnetization on the Toulouse line shows very good qualitative agreement with a recent numerically exact analysis for the isotropic Kondo model obtained from a time-dependent numerical renormalization group study. [7] Therefore, one can expect that the other local dynamical quantities analyzed in this work such as the spin-spin correlation function and the dynamical spin susceptibility also display the main features and that the results presented in this work are qualitatively valid also away from the Toulouse limit.

The relaxation behavior of the spin-spin correlation function, see Eq. (27), is not altered considerably compared to the interaction quench case without magnetic field. Remarkably, the asymptotic long-time behavior of the spin-spin correlation function is universal and its scaling behavior equals the equilibrium case. This universality originates in the property that the asymptotic long-time behavior of the spin-spin correlation function is solely dependent on the low-energy excitations in the vicinity of the Fermi level. By using a simple Fermi liquid argument, it was shown that the only relevant quantity for the prefactor is the local density of states of the quadratic effective

Hamiltonian at the Fermi level.

The dynamical spin susceptibility is not influenced substantially for magnetic fields $h_* < T_K$ smaller than the Kondo temperature and behaves as in an interaction quench scenario without magnetic field. For $h_* > T_K$, one observes a rapid buildup of correlations on a time scale $t_* = 1/h_*$ and damped oscillations appear for times $t > t_*$ that decay on a time scale t_K . The dynamical spin susceptibility shows a maximum whose position roughly scales proportional to the applied magnetic field. Most importantly, the Kondo peak near T_K disappears for sufficiently large h_* indicating that the magnetic field seen by the impurity spin avoids the buildup of Kondo correlations by pinning the local spin thereby suppressing the local spin fluctuations.

In summary we have obtained exact results for the interaction quench dynamics of the Kondo model on the Toulouse line and studied its thermalization behavior. This is a rare case where rigorous results can be found even in non-equilibrium and provides another benchmark in the growing field of non-equilibrium quantum impurity physics. [4, 5, 6, 7, 8, 9, 10, 12]

Acknowledgments

This work was supported through SFB TR12 of the Deutsche Forschungsgemeinschaft (DFG), the Center for Nanoscience (CeNS) Munich, and the German Excellence Initiative via the Nanosystems Initiative Munich (NIM).

Appendix A.

For the evaluation of correlation functions in the macroscopically spin-polarized initial state, it is essential to determine the initial occupation distribution of the spinless fermions

$$f_{kk'} = \langle \psi'_0 | c_k^\dagger c_{k'} | \psi'_0 \rangle \quad (\text{A.1})$$

where the state $|\psi'_0\rangle$ is given by:

$$|\psi'_0\rangle = e^{i\pi\hat{N}_s S_z} e^{i[\sqrt{2}-1]\phi_s(0)[S_z-\frac{1}{2}]} |\psi_0\rangle = e^{iLk_*/8} |\psi_0\rangle \quad (\text{A.2})$$

as the initial state $|\psi_0\rangle$ is an eigenstate of both S_z and N_s . Expressing the modes c_k in terms of the fields $\psi(x)$ and by using the bosonization identity for $\psi(x)$ one obtains:

$$\begin{aligned} f_{kk'} &= \frac{1}{2\pi aL} \int \frac{dx}{2\pi} \int \frac{dx'}{2\pi} e^{-ikx} e^{ik'x'} \times \\ &\times \langle \psi'_0 | e^{i\phi_s(x)} e^{i\frac{2\pi}{L}\hat{N}_s x} e^{-i\frac{2\pi}{L}\hat{N}_s x'} e^{-i\phi_s(x')} | \psi'_0 \rangle \end{aligned} \quad (\text{A.3})$$

Due to Eq. (7), $e^{-i\frac{2\pi}{L}\hat{N}_s x} |\psi_0\rangle = e^{-ik_* x/2} |\psi_0\rangle$ such that:

$$f_{kk'} = \delta_{kk'} \theta\left(\frac{k_*}{2} - k\right). \quad (\text{A.4})$$

Therefore, the initial spin polarized state induces a shift of the chemical potential of the spinless fermionic operators.

References

- [1] D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav and M. A. Kastner, *Nature* **391**, 156 (1998); S. M. Cronenwett, T. H. Oosterkamp and L. P. Kouwenhoven, *Science* **281**, 540 (1998); J. Schmid, J. Weis, K. Eberl and K. von Klitzing, *Physica B* **258**, 182 (1998); W. G. van der Wiel, S. De Franceschi, T. Fujisawa, J. M. Elzerman, S. Tarucha and L. P. Kouwenhoven, *Science* **289**, 2105 (2000).
- [2] G. Toulouse, *C. R. Acad. Sci. Paris* **268**, 1200 (1969).
- [3] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg and W. Zwerger, *Rev. Mod. Phys.* **59**, 1 (1987).
- [4] D. Lobaskin and S. Kehrein, *Phys. Rev. B* **71**, 193303 (2005).
- [5] D. Lobaskin and S. Kehrein, *J. Stat. Phys.* **123**, 301 (2006).
- [6] P. Nordlander, M. Pustilnik, Y. Meir, N. S. Wingreen, D. C. Langreth, *Phys. Rev. Lett.* **83**, 808 (1999).
- [7] F. Anders and A. Schiller, *Phys. Rev. B* **74**, 245113 (2006).
- [8] T. A. Costi, *Phys. Rev. B* **55**, 3003 (1997); M. Plihal, D. C. Langreth and P. Nordlander, *Phys. Rev. B* **61**, R13341 (2000); A. Schiller and S. Hershfield, *Phys. Rev. B* **62**, R16271 (2000); F. B. Anders and A. Schiller, *Phys. Rev. Lett.* **95**, 196801 (2005); H. E. Tureci, M. Hanl, M. Claassen, A. Weichselbaum, T. Hecht, B. Braunecker, A. Govorov, L. I. Glazman, J. von Delft and A. Imamoglu, *arXiv:0907.3854* (2009); I. Affleck and A. W. W. Ludwig, *J. Phys. A: Math. Gen.* **27**, 5375 (1994).
- [9] Z. Ratiani and A. Mitra, *Phys. Rev. B* **81**, 125110 (2010).
- [10] F. Lesage and H. Saleur, *Phys. Rev. Lett.* **80**, 4370 (1998).
- [11] M. Möckel and S. Kehrein, *Phys. Rev. Lett.* **100**, 175702 (2008); M. Eckstein, M. Kollar and P. Werner, *Phys. Rev. Lett.* **103**, 056403 (2009); P. Calabrese and J. Cardy, *Phys. Rev. Lett.* **96**, 136801 (2006); C. Kollath and A. M. Läuchli and E. Altman, *Phys. Rev. Lett.* **98**, 180601 (2007); A. Faribault, P. Calabrese and J.-S. Caux, *J. Stat. Mech.*, P03018 (2009); M. Eckstein and M. Kollar, *Phys. Rev. Lett.* **100**, 120404 (2008); M. Rigol, *Phys. Rev. Lett.* **103**, 100403 (2009); S. R. Manmana, S. Wessel, R. M. Noack and A. Muramatsu, *Phys. Rev. Lett.* **98**, 210405 (2007); M. A. Cazalilla, *Phys. Rev. Lett.* **97**, 156403 (2006).
- [12] A. Komnik, *Phys. Rev. B* **79**, 245102 (2009).
- [13] J. von Delft and H. Schoeller, *Ann. Phys. (Leipzig)* **7**, 225 (1998).
- [14] G. Zarand and J. von Delft, *Phys. Rev. B* **61**, 6918 (2000).
- [15] J. Martinek, Y. Utsumi, H. Imamura, J. Barnas, S. Maekawa, J. Koenig and G. Schoen, *Phys. Rev. Lett.* **91**, 127203 (2003); J. Martinek, M. Sindel, L. Borda, J. Barnas, J. Koenig, G. Schoen and J. von Delft, *Phys. Rev. Lett.* **91**, 247202 (2003).
- [16] D. B. Gutman, Y. Gefen and A. D. Mirlin, *Phys. Rev. B*, 085436 (2010).
- [17] D. Segal, D. R. Reichman and A. J. Millis, *Phys. Rev. B* **76**, 195316 (2007).
- [18] F. Guinea, V. Hakim and A. Muramatsu, *Phys. Rev. B* **32**, 4410 (1985).